

Hexachlorophene
70-30-4 | DTXSID6020690

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 58.4 days

Global applicability domain: Outside

Local applicability domain index: 2.65e-01

Confidence level: 8.54e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>9-Ethyl-9H-fluorene</div> <div>Measured: 2330</div> <div>Predicted: N/A</div>	<div>Image not found</div> <div>Phenanthrene, trimethyl-</div> <div>Measured: 26200</div> <div>Predicted: 75.6</div>	<div>Image not found</div> <div>11H-Benzo[a]fluorene</div> <div>Measured: 88900</div> <div>Predicted: 121</div>
<div>Image not found</div> <div>2-Methylphenanthrene</div> <div>Measured: 1370</div> <div>Predicted: 25.0</div>	<div>Image not found</div> <div>1-Methylpyrene</div> <div>Measured: 33300</div> <div>Predicted: 94.4</div>	